Geoderma 440 (2023) 116713

Contents lists available at ScienceDirect

Geoderma

journal homepage: www.elsevier.com/locate/geoderma

Characterizing uncertainty in process-based hydraulic modeling, exemplified in a semiarid Inner Mongolia steppe

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ARTICLE INFO

Keywords:
Evapotranspiration
Root water uptake
Soil moisture simulation
Uncertainty analysis
Unsaturated hydraulic conductivity

ABSTRACT

Assessing root sources of three uncertainties – parameterization of soil hydraulic characteristics, boundary conditions, and estimation of source/sink terms – is a significant challenge in soil water transport modeling. This study aims to evaluate the uncertainty of three each widely-used parameter estimation methods affecting plot-scale water dynamics. The study employs HYDRUS, a process-based hydrologic model, to incorporate these uncertainties and compare model predictions to measured values in a semiarid Inner Mongolia steppe, China. Soil hydraulic parameters are determined using two direct methods (laboratory-derived approach and evaporation method) and one indirect method (neural network). While each hydraulic parameter method generally simulates soil moisture dynamics, the evaporation method performed better, especially under dry conditions. This suggests that measuring the intensity properties, such as unsaturated hydraulic conductivity, with the evaporation method is crucial for reasonable soil moisture simulation. The study also demonstrates the impact of different applied boundary conditions on simulated soil moisture, specifically the partitioning of reference FAO evapotranspiration via one direct method (soil fraction cover) and two indirect methods (leaf area index and crop height). The partitioning via soil fraction cover reflected a better simulation. Additionally, the study compares the uncertainties of root water uptake function with root growth parameters and constant root depth referenced to grass and pasture, and finds no significant difference among them. Comparing three sources of uncertainty in predicting soil moisture, the study concludes that the input soil hydraulic parameter is more sensitive than evapotranspiration partitioning or representation of root water uptake function. Our study highlights that measuring soil intensity properties can better reflect the effects of land use change, such as compaction, on field water transports.

1. Introduction

Soil water content is a crucial variable for many hydrological and agricultural studies. Numerous numerical models have been developed for predicting soil water dynamics; however, there are still several numerical and conceptual difficulties, e.g., accurate modeling of the root-zone water dynamics (Feddes et al., 1988; Saito et al., 2006, Brimelow et al., 2010). Hydrological simulations require input variables such as soil characteristics, land cover, control structures, and management parameters. This makes the model highly parametrized and uncertain due to the unavailability of most input parameters (Joseph et al., 2018). As a result, modeling soil water transport is challenging when assessing uncertainties which are principally caused by estimating evapotranspiration (Loos et al., 2007), soil properties (Alam et al., 2020), and modeling simplifications (Clark et al., 2016). Improving estimation accuracy requires studying how uncertainty in predictions can be

Abbreviations: LDP, laboratory-derived water retention parameters; NN, neural network analysis; EM, Evaporation method; SFC, soil fraction cover; LAI, leaf area index; Height, crop height; Grass, grass parameters; Pasture, pasture parameters; Growth, root growth parameters; MAE, Mean bias error; RMSE, Root mean square errors; IA, Index of agreement.

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https://doi.org/10.1016/j.geoderma.2023.116713
Received 18 October 2022; Received in revised form 18 October 2023; Accepted 7 November 2023
Available online 16 November 2023

apportioned to different error sources.

Soil hydraulic properties, such as soil water retention, $\theta(h)$, and hydraulic conductivity, $K(h)$, are crucial input parameters in process-based hydrologic models (Christiaens and Feyen, 2001; Peters and Durner, 2008). These soil hydraulic parameters can be obtained using various methods, either direct (e.g., field or laboratory tests) or indirect (e.g., inverse methods or pedotransfer functions) (Šimůnek et al., 1998; Islam et al., 2006). The most widely used direct methods are hydrostatic column experiments to derive $\theta(h)$ and the estimation of $K(h)$ from $\theta(h)$ using capillary bundle models like Mualem's integral (Peters et al., 2015). However, these methods can be time-consuming and impractical for lower water contents. Therefore, the more suitable approach might be the transient flow method, such as multi-step outflow experiments (Durner et al., 1999) or evaporation experiments (Wind, 1968; Šimůnek et al., 1998). In the evaporation method, measurements of the evaporation rate and pressure head at different depths in the soil sample can provide a simultaneous estimation of both $\theta(h)$ and $K(h)$ parameters (Wendroth et al., 1993), either through direct measurements or inverse procedures (e.g., Šimůnek et al., 1998). One recent popular version of the evaporation method involves semi-automated direct measurements using the HYPROP system (Peters et al., 2015; Peters and Durner, 2008; Schindler and Müller, 2006), which is commercialized by the METER group (München, Germany). However, all of those methods assume that the soil remains rigid, which may not always be the case due to changes in volume, height, and diameter that can occur over time due to factors like drying. Thus, all modeling approaches are limited by the rigidity of soil i.e., the internal soil strength range (Horn et al., 2014).

In contrast, various indirect methods have been developed to estimate hydraulic input parameters such as pedotransfer functions (PTFs), especially on a large scale (Schaap et al., 2001). However, the reliability of these methods is still under discussion despite their widespread use. Vereecken et al. (1992) found that estimation errors in hydraulic properties can cause considerable deviations between measured and simulated results. One significant drawback of PTF application is the substantial spatial variability; the location from which parameters are derived may differ from the applied area. Accurate soil moisture modeling depends on the precise specification of site-specific soil hydraulic properties (Brimelow et al., 2010). Although indirect methods are less reliable due to the high uncertainty of parameter estimations, direct methods also have deficiencies due to differences in sample volume, sampling procedures, techniques, and inherent spatial variability, leading to dissimilarities in estimated parameters and modeling applied (Islam et al., 2006).

Soil water transport strongly depends on water availability at the atmospheric boundary. Therefore, understanding the influence of soil hydraulic properties on water simulations must be studied in conjunction with estimating evapotranspiration (ET) and its partitioning (Loos et al., 2007; Ren et al., 2022). Partitioning ET into evaporation (E) and transpiration (T) subcomponents is important for understanding links between ecological and hydrological systems because biological water use is closely coupled with ecosystem productivity. It is widely recognized that plant growth is tightly associated with soil water availability, which in turn influences precipitation water partitioning (Scott et al., 2021). Potential ET can be calculated using various process-based or empirical formulas from meteorological variables, such as the FAO-recommended Penman–Montheith combination equation (Allen, 1998). While ET estimation has been extensively tested and evaluated (Fisher et al., 2005), ET partitioning is relatively lacking and often ignored in modeling. ET partitioning might be a critical boundary condition that significantly impacts water losses (Rana and Katerji, 2000; Eitzinger et al., 2004), especially for models that require the input of potential ET partitioning data, such as process-based hydraulic models like HYDRUS. Usually, potential ET is calculated using meteorological data and vegetation characteristics (Fisher et al., 2005; Loos et al., 2007) and then can be generally partitioned using an empirical beer's law function. However, the sensitivity of different methods related to incorporated parameters lacks a concise evaluation.

Moreover, the ET partitioning model is highly influenced by plant growth dynamics, where the parameterization of water transport can greatly affect the model's accuracy. For instance, Loos et al. (2007) demonstrated that incorporating root water uptake functions into soil water transport models can significantly improve the accuracy of ET partitioning. Two major approaches are used in process-based hydraulic models for simulating root water uptake at the plot or field scale (Hopmans and Bristow, 2002; Fatichi et al., 2016). The *microscopic/mesoscopic* approach considers a single root as an infinitely long cylinder with a uniform radius and water-absorbing properties (Feddes and Raats, 2004). On the other hand, the *macroscopic* approach lumps root water uptake processes into a single sink term in the governing mass balance equation (Šimůnek et al., 2008; Javaux et al., 2008). In most hydraulic models, the *macroscopic* approach is used, and various root water uptake reduction functions have been proposed, ranging from a simple two-parameter S-shaped function (e.g., van Genuchten, 1987) to more complex functions with up to 5 fitting parameters (e.g., Feddes et al., 1978). However, determining the root water uptake parameter remains challenging due to the difficulty in measuring the start or cessation of water absorption by roots. There is a need to assess which root extraction parameter is better suited for inclusion since most hydraulic models assume a relatively constant root distribution function, which is far from reality (Warren et al., 2015).

In Zhao et al. (2010), the accuracy of soil moisture simulations with HYDRUS was validated against in-situ observations from four sites in Inner Mongolia grassland, which varied in grazing intensity. The studies demonstrated that HYDRUS could accurately simulate the dynamics of root-zone soil moisture content at each site during the three growing seasons. However, the study did not comprehensively compare the abovementioned uncertainty in simulating soil moisture. The present study evaluates the uncertainties resulting from soil hydraulic parameters, ET partitioning, and estimation of plant water uptake. To this end, we adopt the functional criteria proposed by Wösten et al. (1986), which are directly related to applications rather than the direct comparison of parameters. Therefore, the accuracy of the functional criteria will serve as the basis for identifying differences between simulated and observed soil moisture dynamics.

Our study aims to assess the uncertainty of various parameter estimation methods commonly used for predicting soil moisture content using the process-based model HYDRUS (Simunek et al., 2008) and identifies potential sources of error. To achieve this, we have proposed a framework that integrates different types of uncertainties stepwise, compares their impacts on the simulation results, and identifies the cause of errors in existing model predictions. Although the parameter estimation methods have been well-tested individually, they have not been previously applied in an integrated manner for water resources or environmental modeling applications.

2. Materials and methods

2.1. The experimental site and measurement

The research site for this study was located in the Inner Mongolia steppe at the Inner Mongolia Grassland Ecosystem Research Station (IMGERS; 43°37′50″N, 116°42′18″E). The selected experiment has been under moderate grazing intensity since 1999. The local climate is continental and semiarid, with a mean annual temperature of 0.7 °C and mean annual precipitation of 343 mm, with more than 85 % of precipitation occurring during the growing season from May to September. The soil is sandy loamy and classified as Calcic Chernozems, according to FAO (2006). According to identified soil horizons (a 20–30 cm thick Ah horizon, followed by an Ach-layer down to 100 cm), undisturbed soil samples (n = 7 for each layer) were generally taken at the four depths of 4–8, 18–22, 30–34, and 40–44 cm. A 100-cm^3 cylinder (inner diameter 5.6 cm, length 4 cm) was used for water retention and conductivity measurements. For the undisturbed soil sample to determine the hydraulic parameters based on the evaporation method, a large-sized cylinder (inner diameter 10 cm, length 6 cm) was used.

Field soil moisture dynamics were monitored from 2004 to 2006 using Theta-probes (Type ML2x, Delta-T Devices, Cambridge, UK) inserted horizontally at 5, 20, and 40 cm depths across three sites. The probes were calibrated for site-specific soil conditions using the gravimetric method and data was recorded at 30-minute intervals by a solar-powered automatic data logger. An on-site meteorological station collected weather data such as precipitation, net radiation, relative humidity, wind speed, and air temperature. Root distribution and root length were determined using the line intersection method in five soil layers: 0–10, 10–20, 20–50, 50–70, and 70–100 cm (Gao et al., 2008) and vegetation parameters such as vegetation and residue cover, leaf area index (LAI), and plant height were also recorded. Vegetation coverage was assessed non-destructively based on Braun-Blanquet (1964), while *LAI* was measured using a leaf-area meter LI-3050 (LI-COR, Nebraska, USA).

Weighing lysimeter experiments were conducted in August 2006 using a device with PVC tubes (20 cm long and 5.4 cm diameter) installed beside the field soil moisture monitoring site. Two treatments, one with grass and the other with bare ground, were applied with three replicates. The evaporation variables were determined using the water balance method with the help of an electronic sensor that weighed the samples hourly.

2.2. Parameter estimation methods

2.2.1. Water retention and hydraulic conductivity functions

In this study, both measurements of retention and conductivity data are fitted by the following van Genuchten-Mualem (VGM) equations (van Genuchten, 1980):

$$S_e(h) = \frac{\theta_w(h) - \theta_r}{\theta_s - \theta_r} = \frac{1}{(1 + |\alpha h|^n)^m} \tag{1}$$

$$K(h) = K_s S_e^l \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \tag{2}$$

where S_e is the effective saturation, θ_s and θ_r are the saturated and residual water contents (L3/L^{-3}(−|-)), respectively; the symbols α (L^{-1}), n, and $m = 1–1/n$ are empirical shape parameters, and the inverse of α is often referred to as the air entry value or bubbling pressure; K_s is the saturated hydraulic conductivity (L/T), and l is a pore connectivity parameter which usually is set to 0.5. The hydraulic soil parameters are summarized in Table 1.

To test the estimation uncertainty of hydraulic parameters, we compared three methods widely used to estimate parameters of the VGM functions: i) laboratory-derived water retention properties (LDP), ii) neural network (NN) analysis, and iii) evaporation method (EM). The soil water retention characteristic for the LDP method is measured with a ceramic pressure plate assembly stepwise desaturating initially saturated samples at equilibrium matric potentials of −1, −3, −6, −15, −30, and −1500 kPa. Seven samples were retrieved from each of the four depths to yield 28 soil cores. K_s was determined with the same-sized cores with a falling head permeameter (Zhao et al., 2010). To convert the former laboratory-measured data to the VGM parameter (Table 1), RETC software (RETention Curve) was employed by a nonlinear least-squares optimization approach to estimate the unknown model parameters from observed retention data (van Genuchten et al., 1991). The fitted VGM parameters were further used to predict the *K(h)* curves based on the VGM equation (Eq. (2)). In the NN method, VGM parameters were derived by pedotransfer functions (PTFs) via the neural network (NN) prediction tool ROSETTA (Schaap et al., 2001) based on data from soil texture and bulk density (Zhao et al., 2010). The EM method is based on the evaporation approach. In a transient flow experiment, the hydraulic conductivity vs. matric potential ratio was determined for undisturbed samples where two microtensiometers and two time-domain reflectometry (TDR) probes were horizontally inserted into the sample from the side through holes in the cylinder at a vertical distance of 3 cm. The sensors continuously recorded the matric potential and water content while the initially saturated sample progressively dried out from the sample surface. The hydraulic conductivity coefficient was calculated from average changes in mean matric potential and water content in short intervals, according to Becher (1970). For more detailed information, please refer to Peth (2004). We used both retention and conductivity data from the evaporation experiment to optimize VGM parameters for the EM method. The measured *K(h)* was compared with the simulated curves based on the fitted parameters of the VGM function using RETC software (van Genuchten et al., 1991).

Table 1
Van Genuchten-Mualem Parameters for the investigated site.

Approach	Soil depth (cm)	θr (cm^3 cm^{-3})	θs (cm^3 cm^{-3})	α (cm^{-1})	n (-)	Ks (cm day^{-1})
LDP	4–8	0.052	0.568	0.020	1.681	46.4
	18–22	0.035	0.529	0.019	1.758	109.6
	30–34	0.045	0.531	0.016	1.710	77.1
	40–44	0.040	0.511	0.017	1.756	63.7
NN	4–8	0.048	0.475	0.018	1.439	64.2
	18–22	0.043	0.451	0.022	1.442	58.9
	30–34	0.040	0.461	0.024	1.454	85.6
	40–44	0.043	0.453	0.025	1.462	72.5
EM	4–8	0.038	0.474	0.005	1.691	46.4
	18–22	0.047	0.453	0.015	1.334	109.6
	30–34	0.050	0.463	0.007	1.942	77.1
	40–44	0.051	0.462	0.008	1.973	63.7

Note: θr = residual water content, θs = saturated water content, α = reciprocal value of air entry pressure, n = the smoothness of pore size distribution and m = 1–1/n. Saturated hydraulic conductivity = *Ks*. LDP: laboratory-derived water retention parameters, NN: neural network analysis, and EM: Evaporation method.

Note that the measured *Ks* were used in the simulation for the LDP and the NN methods. In addition, we did not estimate Ks in the EM method, considering that hydraulic conductivity only can be effectively calculated at a matric potential range of −10 to −90 kPa.

2.2.2. Evapotranspiration partitioning models

The potential evapotranspiration was estimated from the reference FAO Penman-Monteith equation (Allen et al., 1998). Usually, the potential evaporation and transpiration are partitioned based on soil fraction cover (*SFC*) as follows:

$$\begin{aligned} E_p &= (1 - SFC) \times ET \\ T_p &= SFC \times ET \end{aligned} \tag{3}$$

where E_p is evaporation, ET is evapotranspiration, and T_p is transpiration.

Except for the direct measurement of *SFC*, we also calculate *SFC* via Leaf area index, *LAI*, using Beer's law *SFC* = 1-exp(0.463x*LAI*), where exp is the exponential function and 0.463 is the constant for the radiation extinction. *LAI* is determined by: i) directly measured method (abbreviated as *LAI*) and ii) indirectly calculated via the empirically FAO referenced method, i.e., *LAI* (cm^2 cm^{-2}) = 0.24 × crop height (cm) (abbreviated as *height*).

2.2.3. Root water uptake models

The sink term, *S*, corresponds to the volume of water removed from a unit volume of soil per unit time due to the root water uptake (i.e., actual transpiration rate) and can be defined as (Feddes et al., 1978):

$$\Phi(h,z,t) = \beta(h,z,t)\Phi_p(z,t) \quad (4)$$

where $\beta(h,z,t)$ is a prescribed dimensionless response function of the soil water pressure head ($0 \leq \alpha \leq 1$), accounting for the effects of water stress on root water uptake and Φ_p is the potential root water-uptake rate ($L^3 L^{-3} T^{-1}$). With actual local uncompensated root water uptake, $\Phi(z,t) = b(z,t)T_p(z,t)$ where $b(z,t)$ is the normalized water uptake distribution (L^{-1}), and $T_p(t)$ is the potential transpiration rate (L/T). Note that $b(z,t)$ is a function of space and time, allowing to account for plant root growth.

In this study, we initially examined the credibility of critical pressure heads in Feddes' water stress response function were reasonable, which was adapted from grass and pasture (abbreviated as "grass" and "pasture"), respectively (Wesseling, 1991). Under this condition, the root depth and distribution are constant with time. Since we used the same root density distribution function for those two scenarios, the grass and pasture parameters only differed in how they represented the water stress. For the one-dimensional 100-cm soil profile, we set a 90-cm maximum root depth and a linearly decreasing root distribution with depth. The Feddes soil water stress response function was used for all soil depths with the same parameters: $h_1 = -1$ kPa, $h_2 = -2{,}5$ kPa, $h_{3,high} = -20$ kPa, $h_{3,low} = -80$ kPa, and $h_4 = -800$ kPa. The true h_3 parameter was obtained by interpolation between $h_{3,high}$ and $h_{3,low}$, based on the potential evapotranspiration rate, as in the SWATRE code (e.g., Wesseling et al., 1991). Additionally, we compared a root growth method (abbreviated as "growth") with the two root depth-constant methods described above. In this case, the rooting depth linearly increased from 0 cm at the beginning of the growth period to a maximum depth at the date of "full cover" or harvest, which was described by the Verhulst-Pearl model based on our dynamic root measurements (Gao et al., 2008).

2.3. Uncertainty assessment in soil process models

2.3.1. Model setup

The simulations of soil water movement were conducted using HYDRUS-1D (Šimůnek et al., 1998), a finite element model designed for simulating the one-dimensional movement of water, heat, and various solutes in variably saturated media. The program numerically solves Richards' (Richard et al., 2001) equation for saturated and unsaturated water flow. Water content values measured at 5, 20, and 40 cm depths were used as the initial condition across the 0–10, 10–30, and 30–100 cm soil layers. At the soil surface, atmospheric boundary condition was imposed using daily precipitation, potential evaporation (Ep) and transpiration (Tp), and minimum allowed pressure head (cm). Note that fraction-based estimated Ep and Tp in conjunction with the water stress responses (Feddes et al., 1978) for grass and the root growth distribution were used to calculate actual E and T. A free drainage condition was used at the bottom of the domain, assuming that the water table is located far below the area of interest. The soil profile was considered to be 100 cm deep, with observation nodes situated at 5, 20, and 40 cm depths. The simulation period was designed from 1 May to 30 September in both 2005 and 2006, respectively, based on the phenological data from the IMGERS station (Chen and Wang, 2000) combined with our own measurements.

2.3.2. Model implements

The resulting uncertainty due to the different parameters and input data was examined through field-measured moisture data. As addressed before, the soil moisture simulations were subjected to three error sources, e.g., soil hydraulic parameters, ET partitioning, and estimation of plant water uptake. Here, we analyzed those sources in a stepwise manner (Table 2), where the HYDRUS model was employed with three estimation methods (i.e, uncertainties) at each step to compare their performances.

During the first step, three soil hydraulic parameterization approaches (LDP, NN, and EM) were compared. Note that the SFC partitioning boundary condition and "growth" root water function were referenced for this step.

In the second step, three approaches for partitioning ET (SFC, LAI, and height) were compared. The EM method was referenced for the soil hydraulic parameter, and "growth" was referenced for root water function.

In the third step, three approaches for the functions of root water uptake ("grass", "pasture", and "growth") were compared. The EM method was used for the soil hydraulic parameter, and the SFC partitioning boundary condition was referenced.

Consequently, at each step, the dominant role of different uncertainties in simulating soil water dynamics was investigated by quantifying the effects of one factor while fixing the other factor.

2.3.3. Performance evaluation

To assess model predictive performance as compared to observations, we used the following criteria (Brimelow et al., 2010):

(i) the Mean bias error (*MAE*), measuring the average difference between measurements and model:

$$MAE = \frac{1}{n}\sum_{i=1}^{N}(P_i - O_i) \quad (5)$$

(ii) the Root mean square error (*RMSE*), measuring the scatter between measurements and model:

Table 2
Design of the multi-step modeling approaches with three kinds of uncertainties.

step	uncertainty	soil hydraulic parameterization			ET partition			Root water uptake		
		LDP	NN	EM	SFC	LAI	height	grass	pasture	growth
1	1	Y			Y					Y
1	2		Y		Y					Y
1	3			Y	Y					Y
2	1			Y	Y					Y
2	2			Y		Y				Y
2	3			Y			Y			Y
3	1			Y	Y			Y		
3	2			Y	Y				Y	
3	3			Y	Y					Y

Note: LDP: laboratory-derived water retention properties, NN: neural network analysis, EM: evaporation method, SFC: soil fraction cover, LAI: Leaf area index, height: crop height. Y means Yes in the sense it was used.

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2} \quad (6)$$

(iii) the Index of agreement (*IA*), measuring agreement between model and observations:

$$IA = 1.0 - \left[\frac{\sum_{i=1}^{N}(P_i - O_i)^2}{\sum_{i=1}^{N}\left[|(P_i - \overline{O})| + |(O_i - \overline{O})|\right]^2}\right] \quad (7)$$

In the above formula, N is the number of observations, P_i and O_i are the simulated and measured values (i is the data number), and $\bar{O}$ is the mean of the observed series. The *IA* statistic is considered superior to the correlation coefficient in evaluating the accuracy of simulated values (Zhao et al., 2010). *IA* ranges from 0 to 1, with a value of 1 indicating perfect model performance.

3. Results and discussions

3.1. Soil hydraulic parameters in the studied area

In the area we studied, the topsoil had a higher sand content, bulk density, and a lower total carbon content than the subsoil (18 to 44 cm), indicating the presence of pedogenetic stratification. The textural changes in the soil profile influence the total porosity, water retention values, and hydraulic conductivity of the soil horizons. This is consistent with the VGM parameters of the soil horizons (Table 1). Moreover, the parameters α and n based on the EM were largely different from that based on the LDP or NN. Fig. 1 shows large differences in unsaturated hydraulic conductivity function, *K(h)*, among three parameter estimation methods, particularly at moderate dry conditions (the matric potentials ranging between −30 to −90 kPa). This indicates a large discrepancy between the calculated and measured parameters of different estimation methods. One main reason for these differences is that the LDP approach is based on capacity properties, ignoring flow while the EM method considers the transport and thus reflects intensity properties (Horn et al., 2014). Mertens et al. (2004) also reported that using different measurement techniques at the same scale or sample size can yield different Ks estimates.

3.2. Model uncertainty in water flow simulations

3.2.1. Uncertainty of soil hydraulic parameters

The quality of estimated hydraulic parameters was tested by predicting water contents for the two growing periods of 2005 and 2006. There is a general agreement between simulated and measured soil water content for both periods (Fig. 2). Irrespective of the parameter estimation method, an increase in water content in the topsoil after rainfall was well-reflected, indicating that all parameterized models are responsive to input rainfall. The subsoil also showed similar soil moisture dynamics for the simulation period across all model approaches. However, the EM method performed much better in predicting measured soil water values than the other methods. The EM model could almost perfectly simulate water contents at 20 cm depth, while the other two approaches failed to represent field observations adequately. This discrepancy could be due to inaccurate calculated *K(h)* in this layer incorporated in the LDP and NN methods. We also observed large differences in slopes of the *K(h)* for the different estimation approaches at greater matric potential (<−100 kPa) for the 18–22 cm depth compared to the other depths (Fig. 1). Note that between days 130 and 153, the simulation underestimated the water content due to the occurrence of snow (starting on 7th September 2006). This was expected as the current HYDRUS model dose not account for simulating the snow hydrology and frozen soil processes (Zhao et al., 2010).

Our study found that the LDP approach was less accurate in estimating soil moisture profiles under drought conditions, likely due to its reliance on capacity properties. In contrast, the EM method was the most effective in predicting soil moisture profile, as indicated by the lowest *RMSE* and the highest *IA* (Table 3). This method could simulate the natural water flow process, such as soil evaporation physics, under relative drought conditions (Or et al., 2013). Peters et al. (2015) also found that the EM provided more realistic soil hydraulic properties data, especially in the medium to dry moisture range, by accurately accounting for water adsorption flow in incompletely filled capillaries and isothermal vapor flow. However, the LDP approach showed large discrepancies, particularly at the second soil depth, which might not

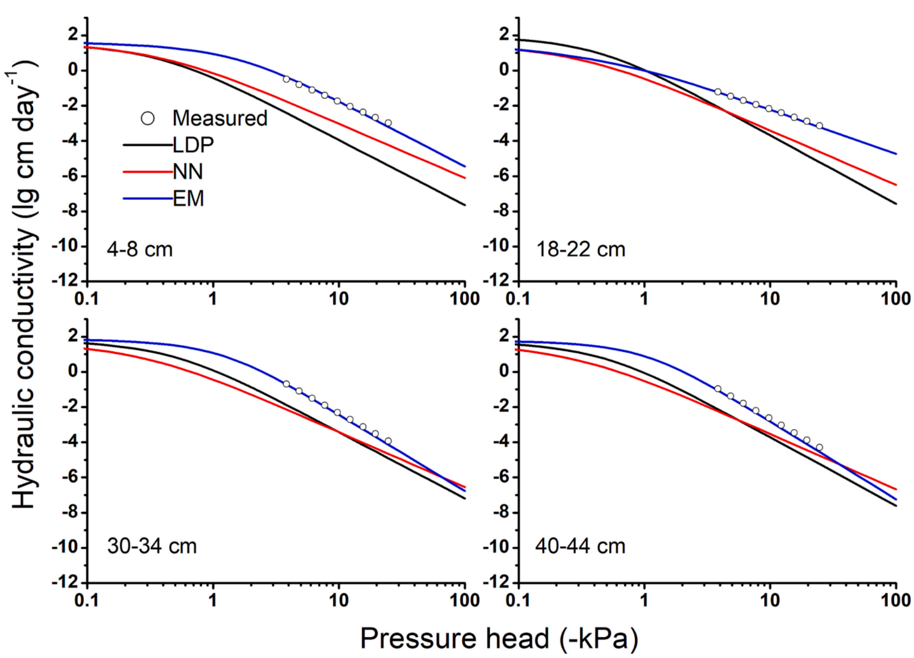

Fig. 1. Comparison of the unsaturated hydraulic conductivity functions derived from three soil hydraulic parameter estimation methods. M: Measured values, LDP: laboratory-derived water retention parameters, NN: neural network analysis, and EM: Evaporation method (the fitting curve is based on the data of the evaporation method).

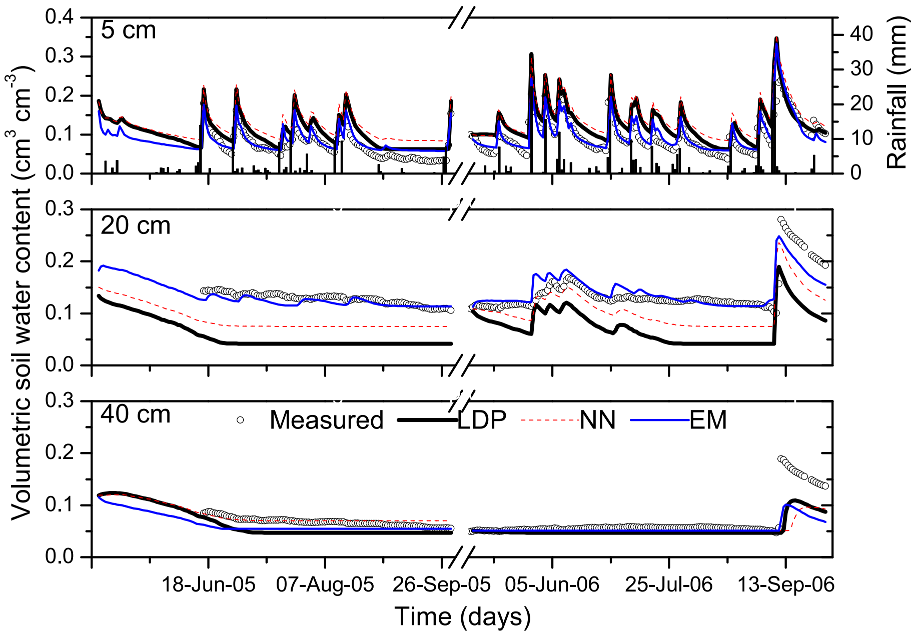

Fig. 2. Comparison of measured and simulated soil moisture dynamics during the growing period between 2005 and 2006 resulting from different soil hydraulic parameter estimation methods: M: Measured, LDP: laboratory-derived water retention parameters, NN: neural network analysis, and EM: Evaporation method (fitting curve based on the data of evaporation method).

Table 3
Statistical values of three simulation approaches for soil moisture dynamics in three soil depths.

Year	Model Appr-oach	MAE 5	MAE 20	MAE 40	RMSE 5	RMSE 20	RMSE 40	IA 5	IA 20	IA 40
		—— cm ——			—— cm ——			—— cm ——		
2005	LDP	−0.028	0.086	0.018	0.032	0.086	0.019	0.828	0.161	0.432
	NN	−0.047	0.052	−0.003	0.049	0.053	0.007	0.688	0.236	0.672
	EM	−0.009	0.007	0.013	0.018	0.010	0.015	0.907	0.738	0.419
2006	LDP	−0.030	0.064	0.014	0.041	0.070	0.026	0.826	0.473	0.756
	NN	−0.044	0.033	0.013	0.050	0.040	0.030	0.776	0.725	0.599
	EM	−0.003	−0.004	0.012	0.023	0.023	0.027	0.935	0.872	0.685
2005	SFC	−0.009	0.007	0.013	0.018	0.010	0.015	0.907	0.738	0.419
	LAI	−0.013	−0.011	0.006	0.019	0.012	0.008	0.893	0.775	0.817
	Height	−0.017	0.006	0.013	0.024	0.013	0.015	0.874	0.593	0.399
2006	SFC	−0.003	−0.004	0.012	0.023	0.023	0.027	0.935	0.872	0.685
	LAI	−0.004	−0.016	0.009	0.024	0.030	0.025	0.925	0.795	0.710
	Height	−0.003	−0.001	0.013	0.023	0.023	0.028	0.938	0.876	0.631
2005	Grass	−0.009	0.007	0.013	0.018	0.010	0.015	0.907	0.738	0.419
	Pasture	−0.016	−0.009	0.010	0.023	0.012	0.012	0.857	0.604	0.462
	Growth	−0.003	−0.005	−0.015	0.018	0.015	0.015	0.897	0.771	0.515
2006	Grass	−0.003	−0.004	0.012	0.023	0.023	0.027	0.935	0.872	0.685
	Pasture	−0.008	−0.016	0.010	0.025	0.030	0.024	0.926	0.795	0.753
	Growth	0.003	−0.001	0.010	0.025	0.023	0.027	0.926	0.876	0.669

Note: MAE = Mean bias error, RMSE = Root mean square errors and IA = Index of agreement. LDP: laboratory-derived water retention parameters, NN: neural network analysis, and EM: Evaporation method, SFC: soil fraction cover, LAI: Leaf area index, height: crop height.

account appropriately for the large pores measured in the laboratory and scale effects related to the sample size. This indicates that site-specific measurement of the water retention data (without the conductivity data) alone may not be sufficient for accurate simulations. The prediction was weakest for the NN method, likely due to the spatial variation of soil properties and the limited accuracy of applied PTFs (Zhao et al., 2010). PTFs introduce substantial spatial variability, and their accuracy outside the development dataset is unknown (Van Looy et al., 2017), leading to potential errors in soil water transport modeling. Our findings suggest that measured *K(h)* is crucial for more confident soil moisture predictions, especially in arid environments (Baroni et al., 2018). Model accuracy was also assessed using *IA* (Table 3), closer to 1 for the EM method, indicating the best goodness-of-fit, followed by LDP and NN (Table 3). This further suggests that the evaporation experiment provides more accurate data than that from pressure plate-measured and using PTFs.

3.2.2. Uncertainty of ET estimation

Based on best-fitting by hydraulic parameters from the EM model approach, we further examined the uncertainty of ET partitioning on model outcomes. Estimating potential T is considered essential for a reliable calculation of soil water in the HYDRUS model. Our findings show that all ET partitioning approaches yield results that reasonably agree with the measured data (Table 3). We found relatively small variations in predicting soil moisture throughout the simulation period, although there are large differences in potential ET estimation from different partitioning methods (Fig. 3). The *SFC* fitted the measured water contents better than the other two (i.e., *LAI* and *height*), especially for the second soil depth. This suggests that reference FAO ET and its partitioning methods suit our study. It is widely accepted that vegetation surface coverage significantly influences the interaction between the vegetation surface and the atmosphere. *LAI* is usually considered a crucial parameter for global, regional, and even small-scale models of the biosphere or atmosphere. A set of exponential equations was fitted to experimental LAI data, which is initially zero or very small, increases exponentially during early vegetative growth, and remains at a plateau until maturity (Islam et al., 2006). However, our study indicated that *LAI*-based prediction is not as good as *SFC*-based predictions for ET partitioning.

Evapotranspiration is the driving force in the water balance, and the current modeling approach intends to distinguish between different ET partitioning methods. Suppose the model strongly under/overestimated potential T. In that case, discrepancies may arise between the simulated and measured flux terms due to the non-linear relationship between soil water contents and *K(h)*. Regardless of the upper boundary applied, the model was able to simulate the general trend of field water content observations, suggesting that the ET partitioning method may not be very sensitive in simulating soil moisture dynamics. However, these findings may only be effective in dry conditions where potential E is much higher than water availability from the soil, and thus the amount of potential E becomes insignificant. This also indicates the minimum allowed pressure head parameter used in the HYDRUS model has correctly distinguished between atmosphere-controlled and soil-limited ET. Note that our comparison did not include an assessment of ET estimation, as we generally consider the ET calculated following the Penman-Monteith equation to be accurate and reasonable (Mastrocicco et al., 2010), while the partitioning of ET remains uncertain and questionable. Soil moisture is crucial in calculating actual ET from potential ET. Both years showed the potential ET is similar to the actual one at the beginning of the summer when soil moisture was available. However, as soil moisture declined throughout the summer, potential ET overpredicted the measured values (Fisher et al., 2005).

3.2.3. Uncertainty of root extraction function

In addition, we assessed the uncertainty associated with root water uptake, which is typically overlooked due to the lack of direct root measurements and challenges in determining the root water uptake function. Existing root water uptake models primarily consider rooting depth and vertical root distribution (Warren et al., 2015). Notably, while these features are treated as static in the grass and pasture approaches in HYDRUS, they are dynamic in the growth approach. Interestingly, we observed no significant differences in moisture predictions across different approaches, including when a root growth model with a highly contrasting water uptake function was considered (Fig. 4). Model efficiency was similar across all approaches (Table 3), which could be attributed to the HYDRUS-1D model's architecture. Specifically, transpiration is determined by the potential T and root water uptake functions. Thus, when the potential T greatly exceeds the necessary root water uptake, the specific type of water uptake function may not significantly impact model outputs.

Our findings align with Hupet et al. (2002), which demonstrated that root parameters do not greatly affect soil water content. Musters et al. (2000) also illustrated that uncertainties in measured soil water contents were considerably higher than uncertainties in root water uptake parameters and that uncertainties in uptake parameters had minimal impact on soil water simulations. The water uptake model reported by Feddes and Raats (2004) indicates that water stress begins when the soil water potential falls below field capacity (e.g., −30 kPa), gradually intensifying until the permanent wilting point is reached. This may explain the low sensitivity of root parameters in areas where water stress is present, as root zone water fluxes are typically low due to the very low unsaturated hydraulic conductivity. Thus, our results suggest that

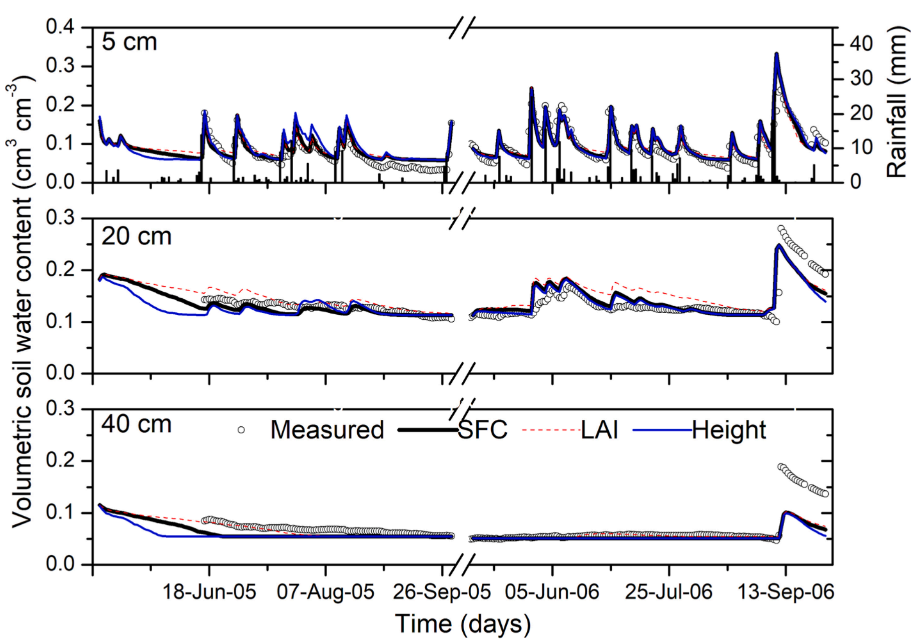

Fig. 3. Comparison of measured and simulated soil moisture dynamics during the growing period between 2005 and 2006 employing different estimation approaches for the evapotranspiration boundary condition. M: Measured, SFC: soil fraction cover, LAI: leaf area index, and Height: crop height.

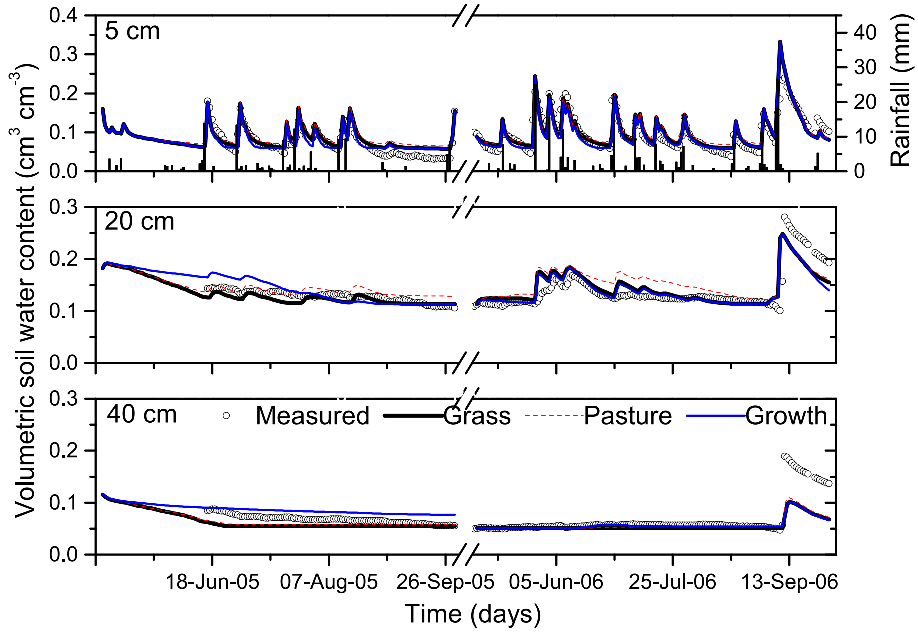

Fig. 4. Comparison of measured and simulated soil water content dynamics during the growing period between 2005 and 2006 employing different estimation methods of root water uptake. M: Measured, Grass: grass parameters, Pasture: pasture parameters, and Growth: root growth parameters.

differences in root water uptake estimation approaches may not be significant during extended droughts when transpiration fluxes are generally reduced. This is consistent with numerous other findings indicating that root water uptake is mainly governed by root distribution and water stress factors during wet periods, whereas the soil water potential and related hydraulic conductivity are the primary drivers during dry periods (Carminati et al., 2016). Besides, a recent sensitivity analysis showed that parameters such as the maximum rooting depth had a minor impact on soil water dynamics and could be specified using literature values without significantly increasing prediction uncertainties (Hartmann et al., 2018). Nevertheless, while our study used a root growth function to estimate root-zone water dynamics, further research is needed to validate root distribution and determine root parameters.

3.2.4. Further model validation by measured ET data

In addition to validating the model with measured soil water data, it is important to quantify the uncertainty using actual ET measurements. The uncertainty analysis of water transport models may show that flux-based data is better suited than content-based data (Ren et al., 2022). Similarly, the results showed that EM-based hydraulic parameters and SFC-based boundary condition are more accurate and suitable for estimating the ET and T than other approaches (Fig. 5). However, all model approaches overestimated ET, which may be because the model and parametrization processes reflect the reinforced hydrological cycles under drought conditions, despite the reliability of our measurement. This requires further investigation.

3.3. Implications for water transport simulation

3.3.1. Importance of soil hydraulic parameters

This study proposes a methodology to evaluate effective soil parameters for modeling the soil moisture content in the unsaturated zone. The EM method was found to best predict soil moisture regimes due to its ability to account for transient flow conditions, unlike the LDP method which is based on equilibrium conditions. This allowed for accurate estimation of real field water flow. During the rainy season (May to July), soil moisture decreased with increasing soil depth, indicating limited water infiltration into deeper soil layers. In contrast, a reverse trend was observed during the dry season (August to September). In the intermediate-depth layers (10–20 cm), soil water contents were significantly greater, suggesting that more rainfall water was stored in this layer. Compared with the EM model, the LDP model was inferior in reflecting water flow in the field (e.g., soil water content at 10–20 cm layers), as it relies on the capacity properties like water retention characteristics. This confirms previous findings of Børgesen and Schaap (2005) that the measurement of *K(h)* is essential to improve soil hydraulic parameter predictions. The study also suggests that when process-based modeling techniques are used, measured input parameters determined in transient flow experiments are essential and outperform parameter estimations based on static experiments in reflecting the field-scale water dynamics. Additionally, the NN method showed the weakest prediction, highlighting the need for suitable extrapolation and upscaling techniques to capture soil spatial variation (Van Looy et al., 2017).

Various reasons may explain the differences between effective and measured parameters. The first is the 'scaling problem', which refers to the fact that the measured parameters may not be appropriate for the model scale, e.g., using small-scale laboratory-estimated *θ(h)* to describe large-scale field water content. To address this, it is recommended to estimate and apply soil hydraulic properties on the same scale (Abbasi et al., 2004). Another factor contributing to differences is the use of different methods to measure the *θ(h)* and *K(h)*, which can result in water flowing in opposite directions (i.e., downwards for *θ(h)* measured using the LDP method and upwards for *K(h)* measured using the EM method). Additionally, porous media are evaluated not only through volume-based measurements and pore distribution, but also through their ability to transmit fluids. Conductivity and permeability are measures of this capability, with conductivity depending on the soil and fluid characteristics and permeability being a pure material property of the porous medium (e.g., pore geometry, ionic strength, and hydrophobicity). Therefore, for our experiment, we found that the EM method provides a better approximation for predicting the wetting front arrival and the shape of the curves than the LDP method. The EM method, which accounts for intensity properties such as soil shrinkage and swelling, reflects the soil structure better for non-rigid soil than the LDP method, which relies on capacity properties (Horn et al., 2014). While other errors in hydraulic parameters, such as high spatial variability of soil

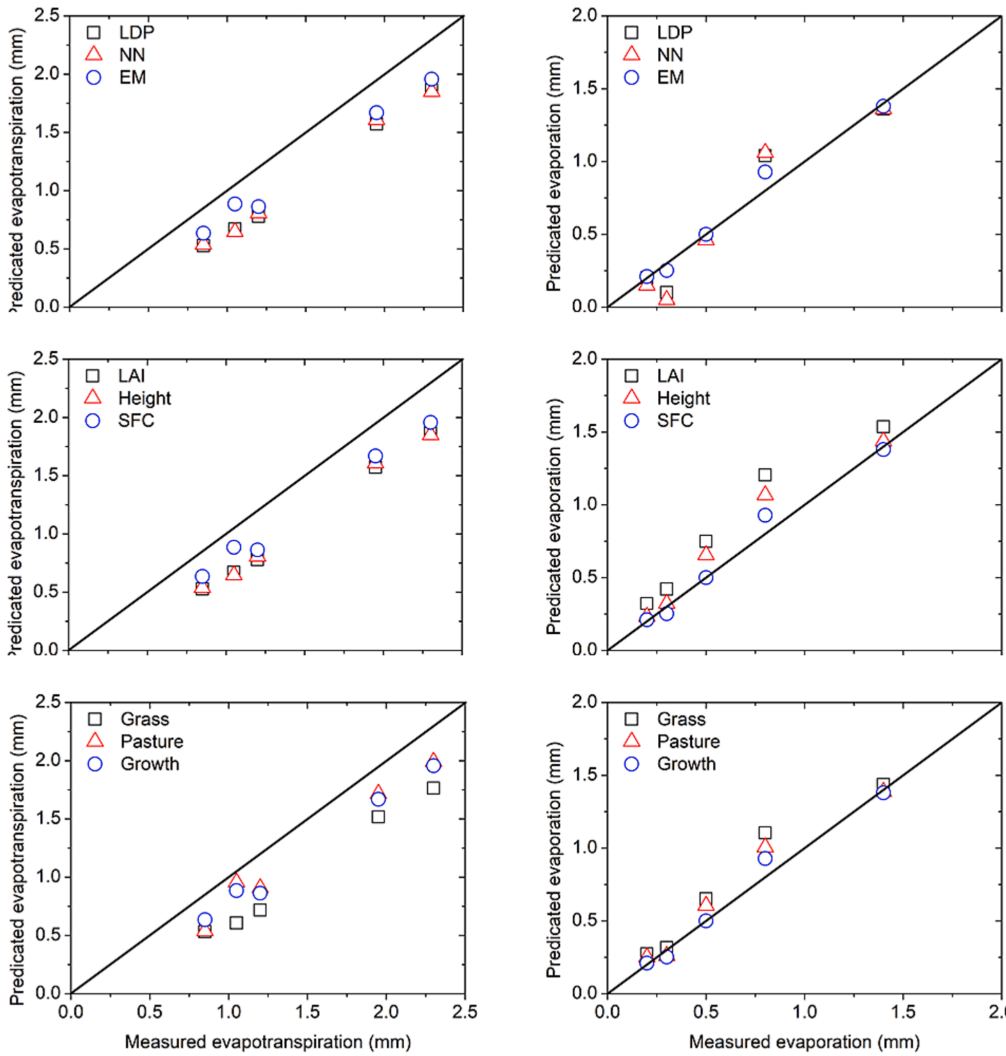

Fig. 5. Comparison of measured and simulated Evapotranspiration/Evaporation during the weighing lysimeter experiment in August 2006. LDP: laboratory-derived water retention parameters, NN: neural network analysis, and EM: Evaporation method (fitting curve based on the data of evaporation method); SFC: soil fraction cover, LAI: leaf area index, and Height: crop height; Grass: grass parameters, Pasture: pasture parameters, and Growth: root growth parameters.

structure, may exist when using pedo-transfer functions, we compared two widely-used parameterized methods from laboratory measurements in this study. We confirmed that more precise, site-specific soil hydraulic properties can be obtained by directly measuring these parameters.

3.3.2. Combined effects from several uncertainties in the process-based model

As demonstrated in this study, assessing uncertainties is crucial for field studies and modeling applications as model uncertainty comparisons are often overlooked. Such knowledge of uncertainties is essential to understand the impact of soil-weather-root interactions. Different approaches for soil hydraulic parameter estimation strongly influence the simulation of soil water dynamics. Our study revealed that the choice of the method for deriving the soil hydraulic parameters, rather than the estimation of the ET method and root water uptake functions, may be more critical when the root zone water content is considered. Understanding the components of ET is crucial for ecohydrological modeling. At higher LAI, transpiration demand increases root water extraction, whereas evaporation from the soil surface becomes negligible. Consequently, partitioning potential ET into actual E and T is important when combining soil water transport models with plant growth functions. Furthermore, although our study found that the root water uptake function is not sensitive in predicting soil water dynamics, it does not imply that root parameters are insignificant. Our findings are based on the model architecture used (dos Santos et al., 2017). In HYDRUS, the conceptualization of the root distribution and water uptake function may not accurately capture the real root-water relation, as it assumes that soil hydraulic properties mainly influence root development under suboptimal conditions. Developing more realistic one-dimensional reduction functions that combine soil and root hydraulic properties, such as the R-SWMS model, seems promising, particularly with the latest advances in noninvasive techniques for root parameterization (Javaux et al., 2008). Understanding roots and their functioning is critical for predicting climate change impacts on terrestrial ecological systems (Feddes and Raats, 2004) and driving new research in this area.

More attention needs to be given to quantifying errors in input variables, parameters, and model architecture. Model outputs should be accompanied by accuracy measures and realistic assessment of model uncertainties to ensure their reliability (Christiaens and Feyen, 2001). The uncertainty in ET partitioning has important implications for water and heat exchange predictions between the land surface and atmosphere. As plants can extract water more efficiently from deeper soil levels than the evaporation process, the timescale over which T declines during a dry spell is much longer than that of the evaporation process (Vereecken et al., 2016). Therefore, the best prediction throughout the growing period is achieved by combining the hydraulic parameters from the EM method, ET partitioning by SFC, and root growth function. While simple approaches like HYDRUS use root length density to approximate uptake capacity, more detailed analyses involve root hydraulic architectures to consider differences in root hydraulic properties between different root orders. However, implementing and parameterizing such detailed analyses in terrestrial system models remains challenging (Couvreur et al., 2012). While adjusting soil hydraulic properties separately for each modeling scenario could lead to a better agreement between measured and simulated moisture dynamics (Zhao et al., 2010). However, it was not done here as we aimed to compare the effects of different hydraulic approaches to predict soil water dynamics. However, relaxing the assumptions and simplifications could strengthen the argument for measuring soil water characteristics. Additionally, it is important to note that hydrological model parameters usually have interactions or correlations, leading to significant joint effects on the output variables (Song et al., 2015). Future studies may address these uncertainties by employing cross-validation or ensemble model approaches.

3.3.3. *Credibility of process-based model*

Our results show that when boundary conditions and root functions are properly chosen, the soil water retention curves can effectively capture the impacts of climate and landuse changes on plot-scale hydrological response. While our investigation of three sources of errors may account for a large portion of the model's uncertainty, other sources, such as model architecture and representativeness error, could still be significant. Nevertheless, this highlights the relatively straightforward process of quantifying uncertainty in model inputs and parameters compared to assessing structural uncertainty in models. The HYDRUS-1D model, widely used for simulating soil water dynamics, requires few input parameters for calibration and has produced satisfactory results in past studies. However, few studies have evaluated uncertainty in HYDRUS-1D simulations, particularly regarding ET partitioning. One survey by Sutanto et al. (2012) explored the potential of HYDRUS-1D to estimate ET partitioning using isotope measurements and the water balance equation. However, this study was only conducted in a laboratory setting and did not produce conclusive partitioning results, indicating the need for further validation using field data.

Root water uptake is a critical process considered in numerical models that simulate soil water content and fluxes in the subsurface, as it controls water flow and recharge to the groundwater. However, most models still use a constant maximum soil-root conductance value for the entire soil-root system instead of coupling soil water transport models with plant root growth dynamics to quantify water balance components (Ryel et al., 2002). A root growth module was developed and implemented into HYDRUS-1D to address this. The HYDRUS software now allows for deriving root growth and water stress functions from laboratory or field experimental data, which can improve the predictions of root water uptake, affected by cardinal temperatures (Hartmann et al., 2018). However, the current root water uptake function may not fully reflect the mechanisms by which the root absorbs soil water, such as characterizing soil water availability related to root distribution (Wu et al., 2021). The stem-root flow parameterization scheme may provide a better alternative (Javaux et al., 2008). The mechanisms driving root water transport dynamics are still widely unknown and technically challenging to capture in situ conditions (Carminati et al., 2016). To reduce uncertainty in the parameterization of root water uptake processes, advances in experimental methods are required, and stable isotopes may provide an excellent tool for studying root permeability, plant adaptation to water availability, and genotype on the uptake and solute transport at small scales or short-term sub-daily timescales (Volkmann et al., 2016; Javaux et al., 2008).

Reliable and accurate uncertainty analysis is crucial for understanding the causes and consequences of error sources, which can help identify alternative ways of managing soils. Our findings differ significantly from other investigations that found input hydraulic parameter uncertainty less than multi-climate ET estimation uncertainty (Joseph et al., 2018). A comprehensive sensitivity analysis for the sink term showed that the maximum root depth controls catchment-scale ET and streamflow (Hartmann et al., 2018). However, the comparison variables chosen may influence our uncertainty assessment, such as soil moisture data and ET data (Baroni et al., 2018). Nevertheless, all model approaches showed similar trends in predicting soil moisture or ET values. We caution that this may only apply to dry conditions and requires further investigation in wet conditions.

4. Conclusions

This study has identified the factors that contribute to the uncertainty in root-zone water simulations. The results indicate that the current modeling uncertainty analysis effectively distinguishes various hydraulic parameters, ET partitioning, and root water uptake parameters. The study proves that incorporating intensity properties such as k(h) in model parameter estimations leads to more accurate predictions. Regarding ET partitioning, the SFC method outperforms the empirical LAI and height approaches, suggesting that direct surface coverage measurement should be used instead of the traditional LAI approach. Additionally, the uncertainty caused by choice of the "correct" ET partitioning appears larger than the differences between root water uptake functions. As a result, these findings could improve our understanding of the factors that regulate soil moisture, particularly regarding the impacts of climate and land use change on field water balance.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgments

This work was supported by the Natural Science Foundation of China (41977009), the Taishan Scholars Program, China (201812096), the Cooperation Project of Key Laboratory of Chinese Academy of Sciences, and the German Research Council (DFG) in the framework of the Interdisciplinary Research Project MAGIM (*Matter fluxes in grasslands of Inner Mongolia as influenced by stocking rate*), and the Key Program of the National Natural Science Foundation of China (42320104006).

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